CLASSIFICATION OF INDIAN COALS FOR COMBUSTION

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1. INTRODUCTION

In annual coal production India ranks fourth in the world, behind China, USA and Russia, with an estimated production of 225 million tons in 1995-96. The utilities burn nearly 60% of the mined coal while industries consume 25-30% of the coal for captive power generation and process heat. The remaining 10-15% goes for the production of coke and miscellaneous applications. Combustion is thus the most important use of coal in India or for that matter, anywhere in the world.

Countries like USA have national coal sample banks and databases. The Pennsylvania state (PENN) coal sample bank and database are well known, which are also used by the US Department of Energy(DOE). The Argonne National Laboratory has used 200 samples from the PENN coal database and using cluster analysis, has identified 8 representative samples among American coals. Similar exercises have been carried out by Illinois Coal Development Board, US DOE's Pittsburgh Energy Technology Center and several universities. The need for a similar coal data bank/database for India and the lack of it at present have been highlighted by Nandakumar and Gopalakrishnan (1988). Especially, for the design of combustion equipment, it will be highly helpful if one can come up with a set of typical Indian coals.

Classification schemes have similar objectives. However, a classification system meant exclusively for combustion applications or for Indian coals does not exist nor is it likely to be developed with the present approaches. Many classification schemes restrict themselves to two or three coal properties but the picture is not complete. If too many properties are involved, classification gets complicated and ends up as a coding scheme. In general, rank, calorific value, proximate and ultimate analyses, fuel and atomic ratios and petrography seem to be the most important variables for characterizing a coal's combustion behaviour. They are highly inter-related, as revealed in the literature. Is it possible to develop a classification system using all these properties and still achieve a reasonably simple grouping? Principal component analysis (PCA) offers a solution, under certain conditions.

2. PCA METHODOLOGY

Principal Component Analysis(PCA) consists of finding an orthogonal transformation of the original variables to a new set of uncorrelated variables, called principal components (PCs), which are derived in decreasing order of importance (Chatfield and Collins, 1980). The usual objective of the analysis is to see if the first few components account for most of the variation in the original data. If they do, then the dimensionality of the problem is reduced. With two PCs, plotting the values in a graph can reveal some patterns in the data.

To validate this proposition, a reference dataset, preferably non-Indian (to avoid biases) and fairly well structured, is needed. Hensel (1980) has used a reference table of US coals for studying combustion and classification and this table will be used for the comparisons. Leaving out lignite-B, of which there are no known reserves in USA or Canada, Hensel has selected eight to eleven coals for each of the remaining 12 groups in the ASTM ranks containing a total of 119 samples. The table contains the Calorific value (Cvd), proximate analysis (Fd and Vd) and ultimate analysis (Cd, Hd, Od, Nd, Sd) on a dmmf basis, to which F/V, C/H and CH/O will be added. Petrographic information is not available and hence is left out for the present exercise. Thus the table serves a dual purpose - it covers the entire spectrum of ranks (except lignite-B) and will serve as a good background for the Indian data. It will also help to compare the Indian and US coals.

The analysis can now be gone through in stages. First, one has to decide about the variables. Since Fd and Vd are complementary, one will do. The variables have to be standardised to have unit variance. The correlation matrix is computed next (Table-1). Of the 10 variables listed, Nd and Sd show poor correlation with the other variables. Nd and Sd are relatively outsiders and hence were left out of the analysis.

Table-1 Correlation matrix between variables

	Cvd	Fd	Cd	Hd	Nd	Sd	Od	F/V	C/H	CH/O
Cvd	1.00	0.71	0.89	–0.30	0.11	0.14	–0.95	0.30	0.40	0.71
Fd	0.71	1.00	0.93	–0.84	–0.34	–0.12	–0.85	0.74	0.84	0.93
Cd	0.89	0.93	1.00	–0.65	–0.16	–0.05	–0.97	0.63	0.73	0.90
Hd	–0.30	–0.84	–0.65	1.00	0.55	0.19	.51	–0.90	–0.96	–0.78
Nd	0.11	–0.34	–0.16	0.55	1.00	0.04	.04	–0.53	–0.53	–0.29
Sd	0.14	–0.12	–0.05	0.19	0.04	1.00	–0.13	–0.16	–0.17	–0.05
Od	–0.95	–0.85	–0.97	0.51	0.04	–0.13	1.00	–0.50	–0.60	–0.85
F/V	0.30	0.74	0.63	–0.90	–0.53	–0.16	–0.50	1.00	0.97	0.73
C/H	0.40	0.84	0.73	–0.96	–0.53	–0.17	–0.60	0.97	1.00	0.81
CH/O	0.71	0.93	0.90	–0.78	–0.29	–0.05	–0.85	0.73	0.81	1.00

The eigen values of the reduced correlation matrix are calculated (Table-2).

Table - 2 Eigen values

	1	2	3	4	5	6	7	8
value	6.26	1.41	0.17	0.09	0.03	0.02	0.01	0.00
%	78.24	17.64	2.17	1.13	0.37	0.29	0.12	0.04
cumulative%	78.24	95.88	98.06	99.19	99.56	99.84	99.96	100.00

The first two eigen values alone are significant and account for nearly 96% of the information. The eigen vectors were next worked out and used to transform the variables to principal components (PC). The PCs corresponding to the first two eigen values for all the samples were plotted in a graph (Figure-1a). **Alphabets are used as symbols and follow the rank**. Thus 'A' refers to meta-anthracite and 'L' refers to lignite-A.

This curve is comparable to the Seyler graph in the sense that with two (pseudo) properties, it enables one to compare several coals. It has in fact captured the essence of all the eight chosen coal properties. The clustering of coals of the of same rank is clearly visible in the figure as also the smooth transition from meta-anthracite at one end to the lignites at the other end. Anthracites and low volatile bituminous coals fall on one side. The high volatile coals and lignites fall on the other side. The medium volatile bituminous coals are near the peak. **This is a new discovery and has not been reported in literature so far.** The graph does not change if mean values alone are used (Figure-1b)

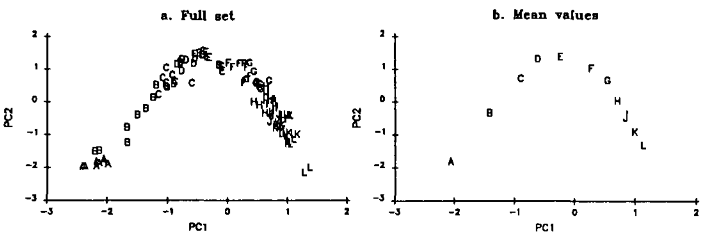

Figure - 1. Principal Components - ASTM Coals

To explore the relationship between PCs and the variables, PC1 and PC2 were plotted against the other variables. The graphs display a rank based continuity and the inescapable conclusion is that the PCs represent the rank in essence. Variation of Cv, Cd and F/V with PCs alone are shown to illustrate the point (Figure- 2 & 3).

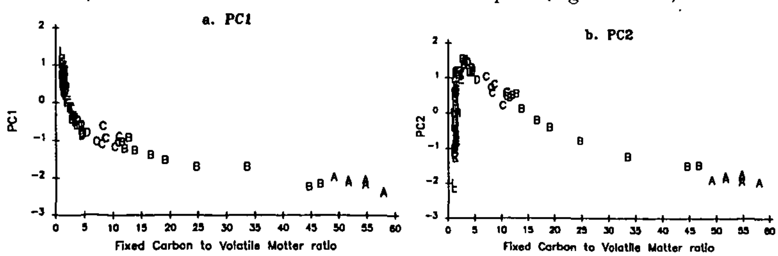

Figure - 2. Principal Components and Fuel Ratio

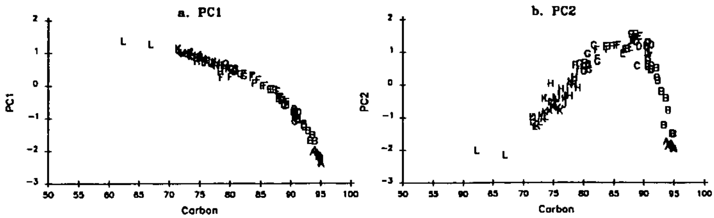

Figure - 3 Principal Components and Carbon

To explore the matter further, the correlations between the original variables and PCs were worked out (Table-3). PC1 is well correlated with all the variables. PC2 however correlates well only with Cvd, Hd, Od, F/V and to some extent with C/H. Significantly, PC3 and the rest show poor correlation with the variables, justifying PCA

Table - 3 Correlation matrix between variables and PCs

	PC 8	PC 7	PC 6	PC 5	PC 4	PC 3	PC 2	PC 1
CV	0.00	0.01	–0.04	0.12	–0.03	–0.11	0.65	–0.74
Fd	0.01	–0.01	–0.09	–0.05	–0.10	0.19	0.01	–0.97
Cd	–0.02	0.07	0.03	–0.07	–0.04	–0.03	0.29	–0.95
Hd	0.02	0.02	–0.05	–0.07	0.11	–0.14	0.50	0.84
Od	0.00	0.06	–0.06	0.06	0.02	0.07	–0.46	0.88
F/V	–0.02	–0.01	–0.06	–0.02	0.07	–0.25	–0.51	–0.82
C/H	0.04	0.02	0.04	0.02	–0.03	–0.10	–0.43	–0.89
CH/O	0.00	0.00	0.01	0.02	0.25	0.17	0.05	–0.95

After a few trials, it was realised that there was a good correlation between PC2 and Hd-Od/8 (HO/8) as well, which appears in the Dulong formula and which can be taken as a measure of the free hydrogen in coal. So, taking HO/8 as an additional variable, step-wise regression analysis between the PCs and the rest of the variables including HO/8 were carried out. The summarised results are presented in Table-4.

Table-4 Step-wise regression analysis

PC1		PC2	
Variable	Multiple Correlation	Variable	Multiple Correlation
Fd	0.971	HO/8	0.956
F/V	0.982	Cvd	0.967
Cd	0.997	F/V	0.999

Function1 = 0.1560 x Fd + 0.1511 x Cd + 0.1317 x F/V
Function2 = 0. 2050 x HO/8 + 0.4603 x Cvd - 0.3621 x F/V

PCs were plotted against the functions which are made up from a combination of the variables appearing in step-wise regression (Figure- 4 a & b).

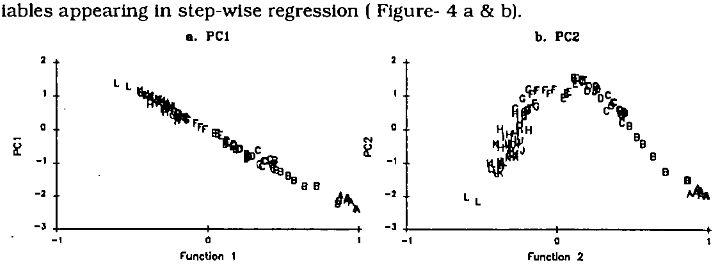

Figure - 4. Principal Components - Correlations

PC1 correlates very well with all the variables but seems to fit best with Fd and Cd. PC2 is highly influenced by HO/8. It is also related to Cvd and F/V to a lesser extent. PC2 vs Function2 resembles the graph PC1 vs PC2. It can be inferred that PC1 and PC2 probably represent Fd/Cd and the available hydrogen. Stated in a different way, it can be inferred that they represent the char and the volatile matter in coal. To probe further into this matter, Seyler's graph was plotted for the original data (Figure-5a) and a modified Seyler's graph was drawn using **Hd-Od/8** (HO/8) instead of Hd (Figure-5b). The shape of the graphs obtained clearly demonstrate that this is the **missing link between the original Seyler graph and the PC graph.** This brings the PCA to an end.

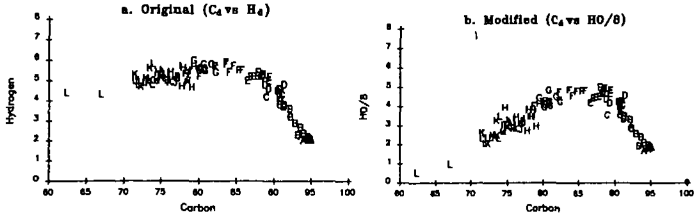

Figure - 5. Seyler Graph - ASTM Coals

3. PCA FOR INDIAN COALS

Twenty major Indian coal fields, based on their reserves were chosen and a statistical sample consisting of nearly 400 records was chosen from the publications of Central Fuel Research Institute's publications (CFRI,1978). The mean properties alone are given in Table-5 for each of these fields.

Table-5 Indian Coals - mean values

Field	Symbol	Cvd	Fd	Cd	Hd	Nd	Sd	Od	F/V	C/H	CH/O	Reserve Million Tons	% to Total
Bisrampur	○	7913	65.7	82.9	4.7	1.6	0.5	10.2	1.9	17.6	9.1	520	0.3
Bokaro	+	8565	70.4	88.2	5.0	2.0	0.6	4.5	2.4	17.7	19.3	9701	5.5
Godavari	⊗	7879	62.0	81.8	4.9	1.7	0.4	11.2	1.7	16.7	7.8	10771	6.1
Ib-River	⌽	7936	62.5	82.8	4.8	1.6	0.5	10.3	1.7	17.2	8.6	20757	11.7
Jharia	ᗜ	8723	74.2	90.1	4.8	2.1	0.6	3.1	3.0	18.7	20.8	19417	11.0
Kamptee	△	7547	62.6	79.9	4.6	1.6	0.3	13.6	1.7	17.4	6.3	1372	0.8
Korba	⧖	7884	63.7	82.8	4.8	1.6	0.5	10.2	1.8	17.4	8.8	8021	4.5
N. Karanpura	∇	8049	63.8	84.1	5.0	1.9	0.7	8.1	1.8	16.8	11.7	13578	7.7
Pench-Kanyan	⧗	8437	63.6	86.0	5.3	1.9	0.5	6.4	1.7	16.1	14.9	1955	1.1
Rajmahal	□	7520	58.9	78.9	4.8	1.7	0.6	13.9	1.4	16.6	5.3	10404	5.9
Ramgarh	⬠	8326	63.0	85.2	5.3	1.9	0.6	7.0	1.7	16.2	11.7	970	0.5
Raniganj	Y	8090	58.8	82.1	5.4	2.1	0.4	9.8	1.4	15.2	8.6	27245	15.4
Singarauli	⊻	7606	60.6	79.8	4.9	1.6	0.6	13.2	1.5	16.4	6.3	9207	5.2
Sohagpur	⍓	8181	65.2	84.4	5.0	1.8	0.5	8.3	1.9	16.9	11.0	2145	1.2
S. Karanpura	⊠	7932	62.4	82.5	5.0	2.1	0.6	9.7	1.7	16.3	8.4	5148	2.9
Talcher	✳	7831	57.7	80.8	5.3	1.7	0.5	11.7	1.4	15.4	7.3	23547	13.3
Wardha	×	7493	59.5	78.7	4.7	1.7	0.4	14.4	1.5	16.6	5.9	4212	2.4
Others	♡	7772	63.5	81.8	4.7	1.7	0.5	11.3	1.8	17.3	7.9	3700	2.1
Tertiary coals	☆	8226	65.9	83.7	5.3	1.3	1.9	8.2	2.9	16.1	15.5	862	0.5
Neyveli lignite	◇	6673	44.1	71.4	5.2	1.1	1.8	22.6	0.8	13.5	3.6	3300	1.9

A similar procedure(normalisation, calculation of correlation matrix, eigen values and eigen vectors) was carried out on the Indian coals. The first two eigen values accounted for more than 90% of the variance (after removal of Sd and Nd). The analysis was carried out on an air-dried basis as well as on a dmmf basis on the 390 random values as well as the 20 mean values. PCs for the Mean values alone are plotted in Figure-6.

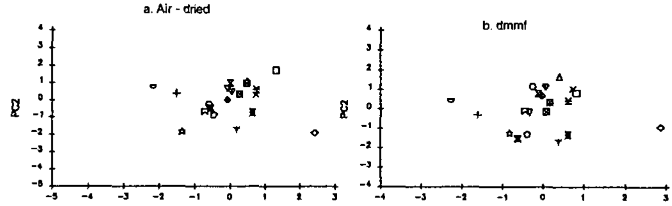

Figure - 6. Principal Components - Indian Coals - Mean Values

Jharia and Bokaro coals and the lignites stood out in both the cases. Rajmahal and tertiary coals looked different on air dried basis but came closer to the other coals on a dmmf basis. It means that their ash and moisture contents are significantly different from the rest. The rest of the samples, in both cases, fell into one small patch. A finer grouping has been done using cluster analysis but that is outside the scope of the present paper. The rest of the analysis and the results were similar to that of the US coals.

4. COMPARISON OF US AND INDIAN COALS

The Indian and US coals were analysed together next. It is worth stressing again that the US data covers almost all the (ASTM designated) ranks and hence serves as a good background. Comparisons are done at two levels- 119 US samples against the 390 Indian random samples at one level and the 12 US (rank-wise) mean values against the 20 Indian (field-wise) mean values at the other level. The same procedure was adopted and the PC graphs are shown in Figure-7. The graphs are exactly similar to Figure -1a and 1b.

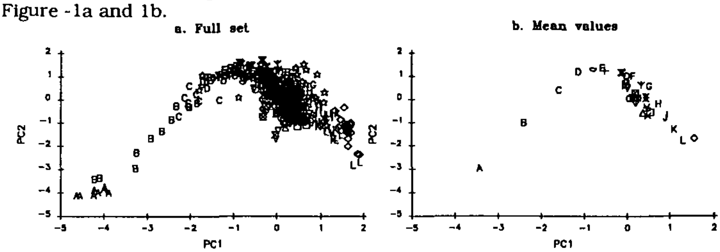

Figure - 7. Principal Components - US and Indian Coals

The 390 Indian samples fall into a small black patch in Figure-7a. A few lignite samples and Tertiary coal samples alone are visible in this graph. In Figure-7b, the Indian lignites fall with the US lignites. Bokaro and Jharia coals have the highest rank among Indian coals. Indian coals fall below the main line for the lower ranks.

The original and modified Seyler graphs were plotted for the 32 mean values (Figure - 8a and 8b). The Indian fields lie below the main graph which dips to the left. The higher oxygen content of Indian coals leads to a corresponding reduction in carbon and hydrogen contents.

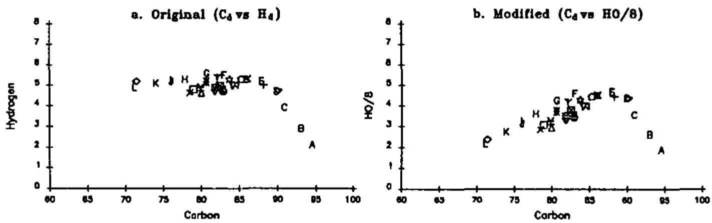

Figure - 8. Seyler Graph - US and Indian Coals - Mean Values

6. CONCLUSIONS

A graph of the principal components can be the new Seyler's graph for coal classification. The PCs seem to represent the rank. The graph shows a peak for the middle ranks. PC1 correlates best with Cd (and Fd) and PC2 with 'Hd- Od/8' (and Vd). PC1 and PC2 seem to represent the carbon and the available hydrogen in coal or broadly, the char and the volatiles of the coal. Among Indian coals, Jharia, Bokaro / Rajmahal/ Tertiary coals/Lignites look different and the rest show little variation. Cluster analysis can reveal a finer distinction.

The PCs are pseudo variables and not physical quantities. The choice of the variables is critical. The graphs at this stage can be used for comparative analyses. The stress is on methodology and the analysis can be repeated for other combinations of variables. There is a good potential for further research.

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